Prediction of Thermophysical Properties Using Fluctuational Thermodynamic Model

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Based on the fluctuational thermodynamic (FT) model we develop a methodology for the prediction of single-phase (including metastable liquid) properties: ρ, h, α_P, K_T, K_S, C_P, C_V and properties of the coexistence (CXS) curve: P_S, ρ_g, ρ_l, r = h_g-h_l based on the knowledge of experimental data of critical parameters (P_c, T_c, ρ_c), triple point (P_t, T_t, ρ_t^l, r_t) and dependence of density $\rho_0(T)$, speed of sound $w_0(T)$ and isobaric heat capacity $C_{P0}(T)$ along one initial supercritical isobar P_0. The FT-model represents the thermodynamic surface by a family of characteristic curves – specific isentropes, for which the simple expressions in parametric form were found. The CXS curve is considered as a smooth continuation of the critical isentrope in terms of the field thermodynamic variables: P, T, μ. We investigated the performance of the proposed methodology on the well-studied fluids (N_2, CH_4, C_2H_4, CO_2, C_6H_{12}) and a reliable description of the single-phase region as well as of CXS curves was found. Due to simplicity of all equations involved in the predictions, the method should be especially attractive for the prediction of phase equilibrium in mixtures based on the known properties of the pure components. A new non-classical (i.e. non-isothermal) concept of the liquid metastability is proposed. It is based on two assumptions: 1) the liquid branch of adiabatic spinodal is the envelope of specific isentropes extended in the region of metastable liquid in the (P,T)-plane; 2) the speed of sound is zero along this curve as well as at critical point. All properties of the adiabatic spinodal in the liquid state have been predicted using data of the CXS curve and initial isobar. Preliminary testing of the proposed method confirmed its reliability and potential applicability for a wide range of practical tasks.